

WHAT IS CLAIMED IS:

1                   1.       A method for preparing a library of compounds, comprising:

- 2                   a) providing a plurality of individual synthesis templates each comprising a solid  
3                         support, wherein said solid support has an interior portion and an exterior  
4                         portion each with a plurality of reactive functional groups, wherein said solid  
5                         support is linked to a scaffold via a scaffold linker, wherein said scaffold has  
6                         at least two scaffold functional groups, and wherein at least two coding tag  
7                         precursors, each comprising a coding functional group and a coding linker, are  
8                         attached to said solid support;
- 9                   b) contacting a first synthesis template with a first reactive component such that a  
10                         first scaffold functional group reacts with said first reactive component to  
11                         afford a first scaffold building block, and a first coding functional group reacts  
12                         with said first reactive component to afford a first coding building block;
- 13                   c) contacting said first synthesis template with a successive reactive component such  
14                         that a subsequent scaffold functional group reacts with said successive reactive  
15                         component to afford a subsequent scaffold building block, and a subsequent  
16                         coding functional group reacts with said successive reactive component to  
17                         afford a subsequent coding building block;
- 18                   d) repeating step c) until said first compound has been prepared; and
- 19                   e) subjecting additional synthesis templates to steps b) - d) with additional reactive  
20                         components to prepare said library of compounds.

1                   2.       The method of claim 1, further comprising the following step:

- 2                   f) cleaving each of said compounds from each of said synthesis templates.

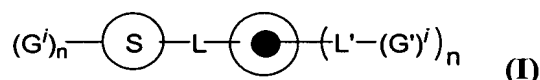
1                   3.       The method of claim 1, wherein the number of said scaffold functional  
2                   groups equals the number of said coding functional groups.

1                   4.       The method of claim 1, wherein said reactive component reacts with  
2                   said scaffold functional group and said coding functional group via a reaction selected from  
3                   the group consisting of amine acylation, reductive alkylation, aromatic reduction, aromatic  
4                   acylation, aromatic cyclization, aryl-aryl coupling, [3+2] cycloaddition, Mitsunobu reaction,  
5                   nucleophilic aromatic substitution, sulfonylation, aromatic halide displacement, Michael  
6                   addition, Wittig reaction, Knoevenagel condensation, reductive amination, Heck reaction,

Stille reaction, Suzuki reaction, Aldol condensation, Claisen condensation, amino acid coupling, amide bond formation, acetal formation, Diels-Alder reaction, [2+2] cycloaddition, enamine formation, esterification, Friedel Crafts reaction, glycosylation, Grignard reaction, Horner-Emmons reaction, hydrolysis, imine formation, metathesis reaction, nucleophilic substitution, oxidation, Pictet-Spengler reaction, Sonogashira reaction, thiazolidine formation, thiourea formation and urea formation.

5. The method of claim 1, wherein said compounds of said library are prepared in parallel.

6. The method of claim 1, wherein at least one of said synthesis templates has a structure of formula I:



wherein

$(G^i)_n$  represents n independent scaffold functional groups,  $G^1$  to  $G^n$ , wherein each  $G^i$  is one of said scaffold functional groups;

$\textcircled{S}$  is said scaffold;

L is said scaffold linker;

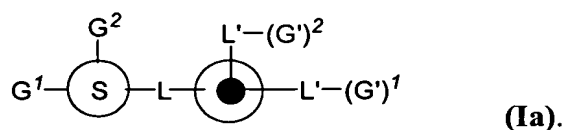
$\textcircled{\bullet}$  is said solid support, wherein the darkened portion represents said interior portion of said solid support, and the lightened portion represents said exterior portion of said solid support;

$(-L' - (G')^i)_n$  represents n independent coding tag precursors, wherein each of said coding tag precursors comprises one of n independent coding functional groups,  $(G')^1$  to  $(G')^n$ , each linked to said solid support via one of n coding linkers, wherein each  $(G')^i$  is one of said coding functional groups, and  $L'$  is said coding linker;

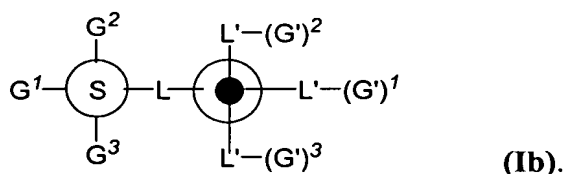
subscript n is an integer from 2 to 10; and

superscript i is an integer from 1 to n.

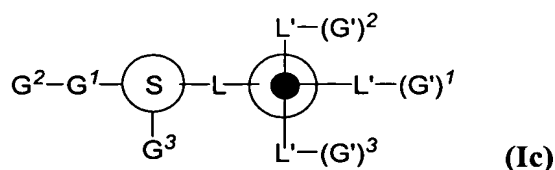
7. The method of claim 6, wherein said synthesis template has a structure of formula Ia:



8. The method of claim 6, wherein said synthesis template has a structure of formula Ib:




9. The method of claim 1, wherein said synthesis template has a structure of formula Ic:




wherein

each of  $\text{G}^1$ ,  $\text{G}^2$  and  $\text{G}^3$  is one of said scaffold functional groups;

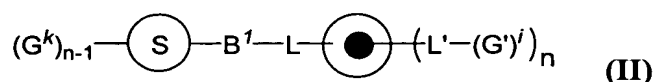
 is said scaffold;

L is said scaffold linker;

 is said solid support, wherein the darkened portion represents said interior portion of said solid support, and the lightened portion represents said exterior portion of said solid support; and

each of  $-\text{L}'-(\text{G}')^1$ ,  $-\text{L}'-(\text{G}')^2$  and  $-\text{L}'-(\text{G}')^3$  is one of said coding tag precursors, each comprising said coding functional group linked to said solid support via said coding linker.

10. The method of claim 1, wherein at least one of said synthesis templates has a structure of formula II:



wherein

$B^1$  represents a first scaffold building block;

$(G^k)_{n-1}$  represents  $n-1$  independent scaffold functional groups,  $G^2$  to  $G^n$ , wherein each  $G^k$  is one of said scaffold functional groups;

$\textcircled{S}$  is said scaffold;

$L$  is said scaffold linker;

$\textcircled{\bullet}$  is said solid support, wherein the darkened portion represents said interior portion of said solid support, and the lightened portion represents said exterior portion of said solid support;

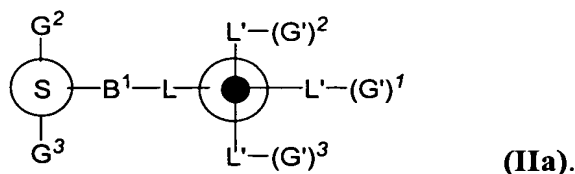
$(L' - (G')^i)_n$  represents  $n$  independent coding tag precursors, wherein each of said coding tag precursors comprises one of  $n$  independent coding functional groups,  $(G')^1$  to  $(G')^n$ , each linked to said solid support via one of  $n$  coding linkers, wherein each  $(G')^i$  is one of said coding functional groups, and  $L'$  is said coding linker;

subscript  $n$  is an integer from 2 to 10;

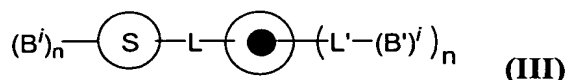
superscript  $i$  is an integer from 1 to  $n$ ; and

superscript  $k$  is an integer from 2 to  $n$ .

11. The method of claim 10, wherein said synthesis template has a structure of formula IIa:




12. The method of claim 1, wherein said steps a) - d) afford a compound template of formula III:




wherein

$(B^i)_n$  represents  $n$  independent scaffold building blocks,  $B^1$  to  $B^n$ , wherein each  $B^i$  is one of said scaffold building blocks;

 is said scaffold;

$L$  is said scaffold linker;

 is said solid support, wherein the darkened portion represents said interior portion of said solid support, and the lightened portion represents said exterior portion of said solid support;

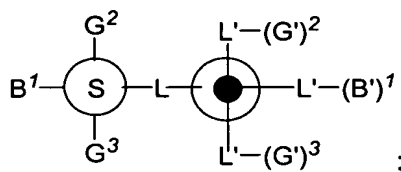
$(-L'-(B')^i)_n$  represents  $n$  independent coding tags, wherein each of said coding tags comprises one of  $n$  independent coding building blocks,  $(B')^1$  to  $(B')^n$ , each linked to said solid support via one of  $n$  coding linkers, wherein each  $(B')^i$  is one of said coding building blocks, and  $L'$  is said coding linker;

subscript  $n$  is an integer from 2 to 10; and

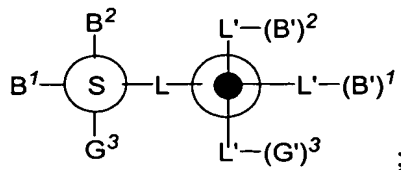
superscript  $i$  is an integer from 1 to  $n$ .

13. The method of claim 1, comprising:

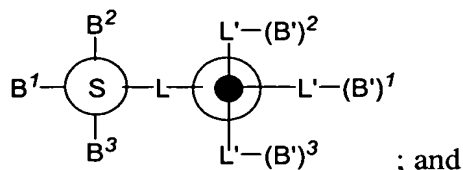
- providing a plurality of individual synthesis templates according to formula Ib;
- contacting a first synthesis template with a first reactive component to afford the following structure:



- contacting said first synthesis template with a successive reactive component to afford the following structure:



d) repeating step c) to prepare said compound attached to the following compound template according to claim 12:



e) subjecting additional of said synthesis templates to steps b) - d) with additional of said reactive components in order to prepare said library of compounds.

14. The method of claim 13, further comprising the following step:

f) cleaving each of said compounds from each of said compound templates.

15. The method of claim 1, wherein, on each of said synthesis templates, each of said scaffold building blocks is encoded by a single coding building block.

16. The method of claim 1, further comprising the following step:

f) decoding each of said compounds by cleaving each of said coding tags from said synthesis template and analyzing said coding tags to determine the identity of said corresponding scaffold building blocks.

17. The method of claim 17, wherein said analyzing is carried out via mass spectrometry.

18. The method of claim 1, wherein said scaffold is the same on each of said synthesis templates.

19. The method of claim 1, wherein at least two different scaffolds are used.

20. The method of claim 1, wherein said scaffold is a member selected from the group consisting of quinazoline, tricyclic quinazoline, purine, pyrimidine, phenylamine-pyrimidine, phthalazine, benzylidene malononitrile, amino acid, tertiary amine, peptide, lactam, sultam, lactone, pyrrole, pyrrolidine, pyrrolinone, oxazole, isoxazole, oxazoline, isoxazoline, oxazolinone, isoxazolinone, thiazole, thiozolidinone, hydantoin, pyrazole, pyrazoline, pyrazolone, imidazole, imidazolidine, imidazolone, triazole, thiadiazole, oxadiazole, benzofuran, isobenzofuran, dihydrobenzofuran, dihydroisobenzofuran, indole, indoline, benzoxazole, oxindole, indolizine, benzimidazole,

9 benzimidazolone, pyridine, piperidine, piperidinone, pyrimidinone, piperazine, piperazinone,  
10 diketopiperazine, metathiazanone, morpholine, thiomorpholine, phenol, dihydropyran,  
11 quinoline, isoquinoline, quinolinone, isoquinolinone, quinolone, quinazolinone,  
12 quinoxalinone, benzopiperazinone, quinazolinone, benzazepine and azepine.

1 21. The method of claim 1, wherein said library of compounds is prepared  
2 via a split-mix methodology.

1 22. A library of compounds prepared by the method of claim 1.

1 23. A library of compounds prepared by the method of claim 2.

1 24. A method for identifying a compound of claim 1 that binds to a target,  
2 said method comprising:

- 3 a) contacting said compound of claim 1 with said target; and  
4 b) determining the functional effect of said compound upon said target.

1 25. The method of claim 24, wherein said biological target is a protein  
2 kinase.

1 26. A method for identifying a compound of claim 2 that binds to a target,  
2 said method comprising:

- 3 a) contacting said compound of claim 2 with said target; and  
4 b) determining the functional effect of said compound upon said target.

1 27. The method of claim 26, wherein said target is a protein kinase.

1 28. A method for preparing a library of compounds, comprising:

- 2 a) providing a population of individual synthesis templates each comprising a solid  
3 support, wherein said solid support has an interior portion and an exterior  
4 portion each with a plurality of reactive functional groups, wherein said solid  
5 support is linked to a scaffold via a scaffold linker, wherein said scaffold has  
6 at least two scaffold functional groups, and wherein at least two coding tag  
7 precursors, each comprising a coding functional group and a coding linker, are  
8 attached to said solid support;  
9 b) splitting said population of synthesis templates into two or more separate pools;

- 10 c) contacting said population of synthesis templates with one or more first reactive  
11 components in said two or more separate pools such that a first scaffold  
12 functional group reacts with one of said first reactive components to afford a  
13 first scaffold building block, and a first coding functional group reacts with  
14 one of said first reactive components to afford a first coding building block,  
15 wherein said contacting step yields subsequent synthesis templates;
- 16 d) mixing said subsequent synthesis templates from said two or more separate pools  
17 into a single pool;
- 18 e) splitting said subsequent synthesis templates into two or more separate pools;
- 19 f) contacting said subsequent synthesis templates in said two or more separate pools  
20 with a successive reactive component such that a subsequent scaffold  
21 functional group reacts with said successive reactive component to afford a  
22 subsequent scaffold building block, and a subsequent coding functional group  
23 reacts with said successive reactive component to afford a subsequent coding  
24 building block, wherein said contacting step yields further synthesis templates;
- 25 g) repeating steps d) - f), wherein said further synthesis templates of step f) become  
26 said subsequent synthesis templates of step d), until said library of compounds  
27 has been prepared.